

Near-Dirichlet quantum dynamics for a p^3 -corrected particle on an interval

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Abstract

We study a nonrelativistic quantum mechanical particle on an interval of finite length with a Hamiltonian that has a p^3 correction term, modelling potential low energy quantum gravity effects. We describe explicitly the $U(3)$ family of the self-adjoint extensions of the Hamiltonian and discuss several subfamilies of interest. As the main result, we find a family of self-adjoint Hamiltonians, indexed by four continuous parameters and one binary parameter, whose spectrum and eigenfunctions are perturbatively close to those of the uncorrected particle with Dirichlet boundary conditions, even though the Dirichlet condition as such is not in the $U(3)$ family. Our boundary conditions do not single out distinguished discrete values for the length of the interval in terms of the underlying quantum gravity scale.

1 Introduction

Several theories of quantum spacetime suggest that low energy corrections due to quantum gravity can be modelled by adding to the conventional quantum mechanical position or momentum operators terms that depend on higher powers of the momentum [1]. Such corrections could be experimentally accessible at low energies through their effects on the spectra of quantum mechanical observables, or through their effects on uncertainty relations. An overview can be found in [1]. A case study with a specific form of the correction terms is given in [2]. A discussion within quantum field theory is given in [3].

In this paper we consider the quantum mechanics of a nonrelativistic particle with a p^3 correction on an interval. The physical motivation to work on an interval of finite length, rather than on the full real line, is to relate the p^3 term to ideas about discreteness

of spacetime: might the coefficient of the p^3 correction, of quantum gravitational origin, single out some discrete values of the interval's length as physically preferred [4]?

A technical issue on the interval is that writing down the Hamiltonian as a differential operator, with or without the p^3 term, does not suffice to define a quantum theory with unitary evolution. What is required is to specify at the ends of the interval boundary conditions that define the Hamiltonian as a self-adjoint operator [5, 6, 7]. Without the p^3 term, the allowed boundary conditions form a $U(2)$ family, which includes as special cases Dirichlet, Neumann and Robin boundary conditions at each of the two ends, but also boundary conditions that relate the two ends, including periodic boundary conditions [7, 8, 9, 10, 11, 12]. With the p^3 term, by contrast, the allowed boundary conditions form a $U(3)$ family [13], within which the uncorrected $U(2)$ family is embedded in a rather subtle way, as we shall show. In particular, the $U(3)$ family does not contain the Dirichlet conditions of the uncorrected theory. Yet it is the Dirichlet conditions that can be regarded as generic in the uncorrected theory, as they tend to ensue when the finite interval is built as the limit of a confining potential without fine-tuning [14].

The following question hence arises. We wish to view the p^3 term as a small correction. Given a choice of boundary conditions within the uncorrected $U(2)$ family, do there exist boundary conditions in the corrected $U(3)$ family for which the effects of the p^3 term remain small, in the sense of perturbative expandability [15]: do the corrected eigenenergies and eigenfunctions approach the uncorrected ones when the coefficient of the p^3 term goes to zero?

The main result of this paper is to show that the answer is affirmative for the Dirichlet boundary conditions of the uncorrected theory, and that the subfamily of $U(3)$ for which this happens is, under certain technical assumptions, indexed by four continuous parameters and one binary parameter. For this subfamily of $U(3)$, the spectrum of the p^3 -corrected theory does however not appear to have structure that would single out distinguished discrete values of the interval's length in terms of the coefficient of the p^3 term.

As an intermediate result, we give an explicit description of the full $U(3)$ family of boundary conditions in the p^3 -corrected theory. The $U(3)$ family is in particular seen to contain the $U(1)$ subfamily of periodicity up to a prescribed phase. Within this $U(1)$ subfamily the p^3 corrections are small in the sense of perturbative expandability, and while this smallness is not uniform over the full set of eigenvalues, we show that the time evolution operator of the corrected theory converges to that of the uncorrected theory in the strong operator topology.

We also show that in the p^3 -corrected theory, boundary conditions independent of the second derivative of the wave function form a $U(1)$ subfamily in which the wave function vanishes at both ends and its first derivative is periodic up to a prescribed phase. Numerical evidence suggests that the eigenenergies within this $U(1)$ subfamily approach the eigenenergies of the uncorrected Dirichlet theory as the coefficient of the p^3 term approaches zero; however, an analytic argument shows that derivatives of the p^3 -corrected eigenfunctions cannot approach those of the uncorrected Dirichlet theory. The

closeness in the eigenenergies with these boundary conditions does hence not extend to closeness in all quantum mechanical observables, in particular in observables involving derivatives.

We begin by introducing in Section 2 the Hamiltonian and writing down its $U(3)$ family of self-adjoint extensions, deferring technical material to two appendices. Relevant facts about the uncorrected Hamiltonian are collected in Section 3. Section 4 discusses two special $U(1)$ subfamilies of boundary conditions, first periodicity up to a prescribed phase, and then conditions independent of the second derivative. The main results about perturbatively near-Dirichlet boundary conditions are given in Section 5. Section 6 presents a brief summary and concluding remarks.

We maintain physical units in that the length of the interval has the physical dimension of length. We however drop an overall multiplicative constant from the Hamiltonian so that energies have units of inverse length squared and reduced Planck's constant \hbar has units of inverse length. The superscript star (*) denotes complex conjugation. The superscript dagger (\dagger) denotes the Hermitian conjugate on matrices and the adjoint on operators.

2 p^3 -corrected Hamiltonian and its self-adjoint extensions

We work in the Hilbert space $\mathcal{H} = L_2([0, L], dx)$, where L is a positive constant with the physical dimension of length. We consider in \mathcal{H} the Hamiltonian operator

$$H = -\partial_x^2 - iqL\partial_x^3, \quad (2.1)$$

where q is a dimensionless positive constant.

For $q = 0$, H reduces to the Hamiltonian of a free nonrelativistic particle. The term that involves q can be thought of as an effective quantum gravity correction, proportional to p^3 [1, 4]. It would be possible to scale L out of the problem by writing $x = Ly$, where $0 \leq y \leq 1$, and working in the Hilbert space $L_2([0, 1], dy)$, but we prefer to keep L in the formulas, in view of potential applications to the underlying quantum gravity context. Note that assuming $q > 0$ is no loss of generality since the sign of q can be changed by the reparametrisation $x \rightarrow L - x$.

We take the domain of H to be initially $\mathcal{C}_c^\infty(0, L)$. H is then densely defined and symmetric. As H and its adjoint H^\dagger are third-order differential operators, the solutions to $H^\dagger\psi = \pm i\psi$ are square integrable on $[0, L]$ and form a three-dimensional vector space for each sign. It follows from von Neumann's theorem that the self-adjoint extensions of H form a $U(3)$ family [5, 6, 7, 13].

To write down the boundary condition that specifies the self-adjoint extensions of H , we note that if ψ and ϕ are smooth functions on $[0, L]$, the condition $(\psi, H\phi) = (H\psi, \phi)$

can be written as $C(u, v) = 0$, where

$$C(u, v) := u^\dagger \begin{pmatrix} G & 0 \\ 0 & -G \end{pmatrix} v, \quad (2.2)$$

$$G := \begin{pmatrix} 0 & i & -q \\ -i & q & 0 \\ -q & 0 & 0 \end{pmatrix}, \quad (2.3)$$

and

$$u = \begin{pmatrix} \psi(0) \\ L\psi'(0) \\ L^2\psi''(0) \\ \psi(L) \\ L\psi'(L) \\ L^2\psi''(L) \end{pmatrix}, \quad v = \begin{pmatrix} \phi(0) \\ L\phi'(0) \\ L^2\phi''(0) \\ \phi(L) \\ L\phi'(L) \\ L^2\phi''(L) \end{pmatrix}. \quad (2.4)$$

In terms of (2.2)–(2.4), the self-adjointness conditions for H are the maximal linear subspaces of \mathbb{C}^6 on which the sesquilinear form (2.2) vanishes [5, 6, 7]. These subspaces are found in Appendix A. We collect here the outcome.

The matrix G (2.3) is Hermitian, and its characteristic polynomial is the cubic

$$P_G(\lambda) = -\lambda^3 + q\lambda^2 + (1 + q^2)\lambda - q^3. \quad (2.5)$$

G has three distinct eigenvalues, which we denote in increasing order by λ_- , λ_0 and λ_+ , and it can be shown that $\lambda_- < 0 < \lambda_0 < q < \lambda_+$. Let

$$(a_1 \ a_2 \ a_3), \ (b_1 \ b_2 \ b_3), \ (c_1 \ c_2 \ c_3), \quad (2.6)$$

be normalised eigen-covectors for respectively λ_- , λ_+ and λ_0 , and let

$$\begin{pmatrix} \rho_1 \\ \rho_2 \\ \rho_3 \end{pmatrix} = \begin{pmatrix} \phi(0) \\ L\phi'(0) \\ L^2\phi''(0) \end{pmatrix}, \quad \begin{pmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \end{pmatrix} = \begin{pmatrix} \phi(L) \\ L\phi'(L) \\ L^2\phi''(L) \end{pmatrix}. \quad (2.7)$$

The self-adjointness boundary conditions for H then read

$$U \begin{pmatrix} \sqrt{-\lambda_-} (a_1\sigma_1 + a_2\sigma_2 + a_3\sigma_3) \\ \sqrt{\lambda_+} (b_1\rho_1 + b_2\rho_2 + b_3\rho_3) \\ \sqrt{\lambda_0} (c_1\rho_1 + c_2\rho_2 + c_3\rho_3) \end{pmatrix} = \begin{pmatrix} \sqrt{-\lambda_-} (a_1\rho_1 + a_2\rho_2 + a_3\rho_3) \\ \sqrt{\lambda_+} (b_1\sigma_1 + b_2\sigma_2 + b_3\sigma_3) \\ \sqrt{\lambda_0} (c_1\sigma_1 + c_2\sigma_2 + c_3\sigma_3) \end{pmatrix}, \quad (2.8)$$

where the matrix $U \in U(3)$ specifies the self-adjoint extension.

Three remarks are in order. First, the notation for the eigen-covectors (2.6) is chosen to avoid complex conjugates in (2.8). The corresponding eigenvectors are the Hermitian conjugates of (2.6) but they will not be needed.

Second, the explicit expressions for the eigenvalues from the cubic solution formula are cumbersome, but it can be verified using (2.5) that if λ is an eigenvalue, the corresponding eigen-covector is proportional to

$$\begin{pmatrix} \lambda(\lambda - q) & i\lambda & q(q - \lambda) \end{pmatrix} . \quad (2.9)$$

Using (2.5) and (2.9) allows us to verify by polynomial algebra identities that will be needed in subsection 4.2, including

$$\lambda_- |a_3|^2 + \lambda_+ |b_3|^2 + \lambda_0 |c_3|^2 = 0 . \quad (2.10)$$

Third, the eigenvalues and the eigen-covectors have small q expansions in non-negative integer powers of q . These expansions are collected in Appendix B.

3 Uncorrected Hamiltonian

In the limit $q \rightarrow 0$, H (2.1) becomes

$$H^{q=0} = -\partial_x^2 , \quad (3.1)$$

and from the small q expansions of the eigenvalues and eigen-covectors of G given in Appendix B it is seen that the boundary condition (2.8) reduces to

$$U_2 \begin{pmatrix} \phi(L) - iL\phi'(L) \\ \phi(0) + iL\phi'(0) \end{pmatrix} = \begin{pmatrix} \phi(0) - iL\phi'(0) \\ \phi(L) + iL\phi'(L) \end{pmatrix} , \quad (3.2)$$

where $U_2 \in U(2)$. $H^{q=0}$ is the Hamiltonian of the free nonrelativistic particle, and (3.2) is its well-known $U(2)$ family of self-adjointness conditions on the interval [7, 8, 9, 10, 11, 12].

Our main interest is in the choice $U_2 = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$, which gives the Dirichlet boundary condition,

$$\phi(0) = \phi(L) = 0 . \quad (3.3)$$

The eigenfunctions are proportional to

$$\sin(m\pi x/L) , \quad m = 1, 2, \dots , \quad (3.4)$$

and the eigenenergies are

$$E_m^{q=0, \text{Dirichlet}} = m^2 \pi^2 L^{-2} , \quad m = 1, 2, \dots . \quad (3.5)$$

We will also be interested in the $U(1)$ family of extensions in which $U_2 = \begin{pmatrix} e^{-i\beta} & 0 \\ 0 & e^{i\beta} \end{pmatrix}$, where $0 \leq \beta < 2\pi$. The boundary condition is

$$\phi(L) = e^{i\beta} \phi(0) , \quad \phi'(L) = e^{i\beta} \phi'(0) , \quad (3.6)$$

which means that the eigenfunctions are periodic up to the prescribed phase $e^{i\beta}$. The eigenfunctions are proportional to $\exp(i(2\pi m + \beta)x/L)$, where $m \in \mathbb{Z}$, and the eigenenergies are

$$E_m^{q=0,\beta} = (2\pi m + \beta)^2 L^{-2} , \quad m \in \mathbb{Z} . \quad (3.7)$$

We note that while the Dirichlet spectrum (3.5) is positive definite, and the spectrum (3.7) is positive definite for $\beta \neq 0$ and positive semidefinite for $\beta = 0$, there exist boundary conditions for which the spectrum is not positive definite, and the ground state energy can be made arbitrarily negative. As an example, consider the $U(1)$ family of extensions in which $U_2 = \begin{pmatrix} 0 & -e^{-i\gamma} \\ -e^{-i\gamma} & 0 \end{pmatrix}$, where $0 \leq \gamma < 2\pi$. The boundary condition is

$$\cos(\gamma/2)\phi(0) = -\sin(\gamma/2)L\phi'(0) , \quad \cos(\gamma/2)\phi(L) = \sin(\gamma/2)L\phi'(L) , \quad (3.8)$$

which includes the Dirichlet condition (3.3) as the special case $\gamma = 0$. When $\gamma = 0$ or $\pi \leq \gamma < 2\pi$, there are no negative eigenenergies. However, when $0 < \gamma < \pi$, there is a negative energy ground state, and when $0 < \gamma < 2\arctan(\frac{1}{2})$, there is also one negative energy excited state: the respective eigenenergies E_0 and E_1 are obtained as the unique negative solutions to

$$\tan(\gamma/2)\sqrt{-E_0 L^2} = \coth\left(\frac{1}{2}\sqrt{-E_0 L^2}\right) , \quad (3.9a)$$

$$\tan(\gamma/2)\sqrt{-E_1 L^2} = \tanh\left(\frac{1}{2}\sqrt{-E_1 L^2}\right) . \quad (3.9b)$$

In the limit $\gamma \rightarrow 0_+$, the two negative eigenenergies disappear by descending to negative infinity, while the rest of the spectrum approaches the Dirichlet spectrum (3.5).

4 Two special $U(1)$ boundary condition families

In this section we consider two special $U(1)$ boundary condition families. The first family is manifestly not close to the Dirichlet condition of the unperturbed theory: instead, it extends the periodicity up to a prescribed phase (3.6) to the perturbed theory, and its purpose is to provide an explicitly solvable example in which both the quantitative and qualitative features of the $q \rightarrow 0$ limit can be analysed. In particular, both the eigenenergies and the eigenstates will be seen to be perturbatively close to those of the unperturbed theory, and the uniformness of this closeness can be characterised in terms of the topology in which the time evolution operator of the perturbed theory converges to that of the unperturbed theory. The purpose of the second family is to show that any boundary condition in which both the eigenenergies and the eigenstates are perturbatively close to those of the unperturbed Dirichlet theory must necessarily involve conditions on the second derivative of the wave function.

4.1 Periodicity up to a prescribed phase

Consider in (2.8) the choice $U = \text{diag}(e^{-i\beta}, e^{i\beta}, e^{i\beta})$, where $0 \leq \beta < 2\pi$. As the eigenvectors (2.6) are linearly independent, (2.8) is equivalent to

$$\phi(L) = e^{i\beta}\phi(0), \quad \phi'(L) = e^{i\beta}\phi'(0), \quad \phi''(L) = e^{i\beta}\phi''(0), \quad (4.1)$$

which means that the eigenfunctions are periodic up to the prescribed phase $e^{i\beta}$. The eigenfunctions are proportional to $\exp(i(2\pi m + \beta)x/L)$, where $m \in \mathbb{Z}$, and the eigenenergies are

$$E_m^\beta = (2\pi m + \beta)^2 (1 - q(2\pi m + \beta)) L^{-2}, \quad m \in \mathbb{Z}. \quad (4.2)$$

From this explicit solution we can make the following three observations.

First, for given m , the eigenenergy E_m^β (4.2) converges to that of the unperturbed theory (3.7) as $q \rightarrow 0$. Also, the corresponding eigenfunction and all of its derivatives converge to those of the unperturbed theory, in (say) the L_2 norm. The $q > 0$ theory with the boundary condition (4.1) is in this sense perturbatively expandable about the $q = 0$ theory with the boundary condition (3.6) [15].

Second, if $q > 0$ is fixed, E_m^β is close to $E_m^{q=0,\beta}$ only for those m for which $|2\pi m + \beta| \ll 1/q$. In particular, for fixed $q > 0$, the spectrum is unbounded both above and below, and the asymptotic behaviour of the large positive and negative eigenenergies is dominated by the p^3 term in the Hamiltonian. The perturbative expandability does hence not hold uniformly over the full set of the eigenvalues.

Third, we may characterise the non-uniformity in the small q behaviour in terms of the time evolution operator $V_t^{q,\beta} = \exp(-i\hbar^{-1}H^{q,\beta}t)$: it is straightforward to verify that for each t and β , $V_t^{q,\beta}$ converges to $V_t^{q=0,\beta}$ as $q \rightarrow 0$ in the strong operator topology but not in the operator norm topology.

4.2 Boundary conditions independent of ϕ''

The boundary conditions for the unperturbed theory involve the values of the wave function and of its first derivative at the boundary, but not the values of the higher derivatives. We now ask: which boundary conditions for the perturbed theory involve only the values of the wave function and of its first derivative at the boundary?

Requiring ρ_3 and σ_3 to drop out of (2.8), and using (2.10), we find that U is given by

$$\frac{1}{(\sqrt{-\lambda_-}|a_3|)^2} \begin{pmatrix} 0 & (\sqrt{-\lambda_-}a_3)(\sqrt{\lambda_+}b_3^*) & (\sqrt{-\lambda_-}a_3)(\sqrt{\lambda_0}c_3^*) \\ (\sqrt{-\lambda_-}a_3^*)(\sqrt{\lambda_+}b_3) & (\sqrt{\lambda_0}c_3)^2\alpha & -(\sqrt{\lambda_+}b_3)(\sqrt{\lambda_0}c_3)\alpha \\ (\sqrt{-\lambda_-}a_3^*)(\sqrt{\lambda_0}c_3) & -(\sqrt{\lambda_+}b_3)(\sqrt{\lambda_0}c_3)\alpha & (\sqrt{\lambda_+}b_3)^2\alpha \end{pmatrix}, \quad (4.3)$$

		$q = 10^{-2}$				$q = 10^{-4}$			
m	m^2	$\beta = 0$	$\beta = \frac{1}{2}\pi$	$\beta = \pi$	$\beta = \frac{3}{2}\pi$	$\beta = 0$	$\beta = \frac{1}{2}\pi$	$\beta = \pi$	$\beta = \frac{3}{2}\pi$
1	1	1.129	1.030	0.9997	0.9440	1.00006	1.00005	1.00000	1.00007
2	4	3.999	3.924	3.889	3.792	4.00000	3.99861	3.98966	4.00189
3	9	9.205	9.079	8.962	8.023	9.00053	9.00046	9.00000	9.00062
\vdots	\vdots	\vdots	\vdots	\vdots	\vdots	\vdots	\vdots	\vdots	\vdots
11	121	84.42	80.03	77.07	75.37	121.001	121.001	120.999	121.002
12	144	92.18	90.36	89.26	87.76	143.999	143.946	143.320	144.063

Table 1: The table shows numerical results for $(L/\pi)^2$ times the 12 lowest positive eigenenergies for $q = 10^{-2}$ and $q = 10^{-4}$ under the boundary condition (4.4) with $\beta = 0$, $\beta = \frac{1}{2}\pi$, $\beta = \pi$, and $\beta = \frac{3}{2}\pi$, enumerated by the index m shown in the first column, and suppressing $m = 4, 5, \dots, 10$ where the pattern continues in a straightforward way. The second column shows $(L/\pi)^2$ times the corresponding eigenenergies $E_m^{q=0, \text{Dirichlet}}$ (3.5) in the $q = 0$ theory with the Dirichlet boundary condition. The data suggests that the eigenenergies are converging to $E_m^{q=0, \text{Dirichlet}}$ as $q \rightarrow 0$.

where the only remaining freedom is in the choice of the parameter $\alpha \in \mathbb{C}$ with $|\alpha| = 1$. It can be verified, using (2.10) and four other similar identities, that (2.8) with U given by (4.3) is equivalent to

$$\phi(0) = \phi(L) = 0, \quad (4.4a)$$

$$\phi'(L) = e^{i\beta} \phi'(0), \quad (4.4b)$$

where $0 \leq \beta < 2\pi$ and $e^{i\beta}$ is proportional to α in (4.3) by a phase that is determined by the phase choices of the eigen-covectors (2.6). (With the phase choices made in Appendix B, $e^{i\beta} = \alpha$.)

The main observation for us is that while the unperturbed Dirichlet wave functions satisfy (4.4a), they do not satisfy (4.4b), even though a subset of them satisfies (4.4b) for $\beta = 0$ and the complementary subset for $\beta = \pi$. This means that the derivatives of the perturbed wave functions cannot converge to those in the unperturbed Dirichlet theory at least near the boundaries. Numerical experiments suggest that as $q \rightarrow 0$ with fixed β , the low-lying positive eigenenergies do converge to the $q = 0$ Dirichlet eigenenergies $E_m^{q=0, \text{Dirichlet}}$ (3.5); sample numerical data is shown in Table 1. This means that as $q \rightarrow 0$, the perturbed eigenfunctions must contain a rapidly oscillating component, with the asymptotic form $\exp(ix/(qL))$, which plays an essential role in satisfying (4.4). A similar rapidly oscillating component can be verified to occur when the p^3 correction is replaced by a p^4 correction [16].

In summary, the boundary conditions independent of the second derivatives cannot yield a theory in which both the eigenenergies and the eigenfunctions are perturbatively expandable at small q in the sense that we are looking for.

For use in Section 5, we record here that when the phases of the eigen-covectors (2.6) are chosen as in Appendix B, the matrix (4.3) has the small q expansion

$$\begin{pmatrix} 0 & -1 + q - \frac{1}{2}q^2 + \cdots & \sqrt{2q}(1 - \frac{1}{2}q + \cdots) \\ -1 + q - \frac{1}{2}q^2 + \cdots & 2q(1 - q + \cdots)\alpha & \sqrt{2q}(1 - \frac{3}{2}q + \cdots)\alpha \\ \sqrt{2q}(1 - \frac{1}{2}q + \cdots) & \sqrt{2q}(1 - \frac{3}{2}q + \cdots)\alpha & (1 - 2q + 2q^2 + \cdots)\alpha \end{pmatrix}. \quad (4.5)$$

5 Near-Dirichlet spectrum at small q

We saw in subsection 4.2 that the Dirichlet condition of the $q = 0$ theory does not generalise in a straightforward way to $q > 0$, where any boundary condition that does not involve ϕ'' must be in the $U(1)$ family (4.4). We now show that when q is positive but small, there is a family of boundary conditions that are close to the $q = 0$ Dirichlet theory in the sense of perturbative expandability of both the eigenenergies and the corresponding wave functions.

We look for solutions to the eigenvalue equation $H\phi = E\phi$ in the form

$$\exp(ir_+x/L) - B \exp(ir_-x/L), \quad (5.1)$$

where $r_- = -m\pi + (\text{corrections in } q)$ with $m = 1, 2, \dots$, $r_+ = (1 - qr_- - \sqrt{1 + 2qr_- - 3q^2r_-^2})/(2q) = m\pi + (\text{corrections in } q)$, and $B = 1 + (\text{corrections in } q)$. The expression for r_+ in terms of r_- comes from the eigenvalue equation, and $E = (r_-^2 - qr_-^3)L^{-2}$. When $q \rightarrow 0$, (5.1) reduces to the $q = 0$ Dirichlet eigenfunction (3.4), and E reduces to $E_m^{q=0, \text{Dirichlet}}$ (3.5). Note that we have excluded from (5.1) a term proportional to the third linearly independent solution to $H\phi = E\phi$, given by $\exp(ir_0x/L)$ where $r_0 = (1 - qr_- + \sqrt{1 + 2qr_- - 3q^2r_-^2})/(2q)$, because r_0 diverges as $q \rightarrow 0$ so that the wave function with this term present would not be perturbatively expandable in q .

We choose the phases of the eigen-covectors (2.6) so that $a_1 > 0$, $b_1 > 0$ and $c_3 > 0$. From the small q expansions given in Appendix B it is seen that the $q = 0$ Dirichlet condition is then obtained from (2.8) by setting $q = 0$ and

$$U = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -s \end{pmatrix} \quad (5.2)$$

where s may be any complex number of unit modulus. We hence look for a $q > 0$ boundary condition in which the matrix U in (2.8) has the form

$$U = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -s \end{pmatrix} U_0, \quad (5.3)$$

where s is a q -independent complex number of unit modulus and the unitary matrix U_0 is the 3×3 identity matrix plus corrections in q .

The formulas in Appendix B show that the q -dependent coefficients in (2.8) have small q expansions that proceed in positive integer powers of $q^{1/2}$. We hence assume that U_0 , r_- and B have expansions that proceed in positive integer powers of $q^{1/2}$. We find that there are exactly two ways to make the expansions consistent to order q^2 . These are as follows:

Case I. Set U_0 to the identity matrix and let s remain arbitrary. To order q^2 , we then find

$$r_- = -m\pi + \frac{1}{2}m^2\pi^2q, \quad (5.4a)$$

$$r_+ = m\pi + \frac{1}{2}m^2\pi^2q, \quad (5.4b)$$

$$B = 1 - m\pi q + \frac{1}{2}m^2\pi^2q^2, \quad (5.4c)$$

$$E = E_m^{\text{pert}} := \left(m^2\pi^2 - \frac{5}{4}m^4\pi^4q^2\right)L^{-2}. \quad (5.4d)$$

The correction in the eigenenergies (5.4d) occurs in order q^2 , which is higher than one might have expected on grounds of the order q term in H . Note that none of the formulas in (5.4) depend on s .

Case II. Set $s = \pm 1$ and

$$U_0 = \exp \left[i \left(k_1 q^{1/2} + k_2 q + k_3 q^{3/2} + k_4 q^2 + O(q^{5/2}) \right) \begin{pmatrix} -1 & s & 0 \\ s & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \right], \quad (5.5)$$

where k_1 , k_2 , k_3 and k_4 are real-valued constants, not all of them vanishing. The expressions (5.4) then acquire additional terms proportional to $q^{1/2}$, q , $q^{3/2}$ and q^2 , with coefficients that involve s and positive powers of k_1 , k_2 , k_3 and k_4 . We record here only the expression for the eigenenergy:

$$\begin{aligned} E = & \left(m^2\pi^2 + 2m^2\pi^2k_1((-1)^ms + 1)q^{1/2} \right. \\ & + 2m^2\pi^2(3k_1^2 + k_2)((-1)^ms + 1)q \\ & + \frac{2}{3}m^2\pi^2[k_1^3(25 - m^2\pi^2) + 18k_1k_2 + 3k_3]((-1)^ms + 1)q^{3/2} \\ & + \left\{ -\frac{5}{4}m^4\pi^4 + \frac{2}{3}m^2\pi^2[2k_1^4(33 - 5m^2\pi^2) + 3k_1^2k_2(25 - m^2\pi^2) \right. \\ & \left. \left. + 9k_2^2 + 18k_1k_3 + 3k_4\right]((-1)^ms + 1) \right\} q^2 \Big) L^{-2}. \end{aligned} \quad (5.6)$$

Three comments are in order. First, note that Case I and Case II are distinct because in Case II we have assumed at least one of the constants k_1 , k_2 , k_3 and k_4 to be nonvanishing. In the limit in which all four of these constants are taken to zero, Case II reduces to Case I with $s = \pm 1$.

Second, neither Case I nor Case II includes any of the ϕ'' -independent boundary conditions (4.4). This can be seen by comparing (4.5) to (5.2) and to (5.3) with (5.5).

Third, neither Case I nor Case II remains consistent when the perturbative expansion is continued beyond order q^2 .

It should be emphasised that while we have shown that there exists a set of eigenenergies and eigenfunctions such that each of them is perturbatively expandable as $q \rightarrow 0$, we have not examined whether there exists a sense in which the expandability might hold uniformly over the full set of eigenenergies. The example of subsection 4.1 suggests that the spectrum for fixed $q > 0$ is likely to be unbounded both from above and from below, the asymptotic behaviour of the large positive and negative eigenenergies to be dominated by the p^3 term in the Hamiltonian, and the expandability not to hold uniformly over the eigenenergy set. The closeness of the time evolution operator of the perturbed theory to that of the unperturbed theory might nevertheless again be characterisable in terms of convergence in an appropriate operator topology; however, verifying such convergence properties would require new techniques for analysing the full set of eigenenergies at fixed $q > 0$.

As a final comment, we note that numerical evidence, shown in Tables 2 and 3, indicates that even within the energy range over which the perturbative formula (5.4d) gives a good approximation to the eigenenergies, there occur occasional intercalating, nonperturbative eigenenergies that are not covered by the perturbative formula. These nonperturbative eigenenergies appear however to become rarer as q decreases.

6 Conclusions

We have discussed the quantum mechanics of a nonrelativistic particle on an interval of finite length when the Hamiltonian contains a correction term proportional to p^3 . We gave an explicit description of the $U(3)$ family of self-adjoint extensions of the Hamiltonian, and we showed that the only boundary conditions that do not involve the second derivative of the wave function require the wave function to vanish at the two ends and its derivative to be equal at the two ends up to a prescribed phase. This implies in particular that the Dirichlet condition of setting the wave function to zero at the two ends does not qualify on its own as a self-adjointness condition.

We saw that periodicity up to a prescribed phase does belong to the $U(3)$ family of self-adjointness conditions. The eigenenergies and eigenfunctions were written down in terms of elementary expressions, and we noted that both the eigenenergies and the eigenfunctions are perturbatively expandable about the limit in which the coefficient of the p^3 correction term vanishes. While the expandability is not uniform over the eigenvalue set, it is sufficiently strong to make the time evolution operator of the perturbed theory converge to that of the unperturbed theory in the strong operator topology, although not in the operator norm topology.

Our main result was to find a subfamily of self-adjointness conditions, indexed by four continuous parameters and one binary parameter, under which there exists a countable set of eigenenergies and corresponding eigenfunctions that are perturbatively close to those of the uncorrected nonrelativistic particle under Dirichlet boundary conditions.

$$q = 10^{-2}$$

m	$L^2 E_m^{\text{pert}} / \pi^2$	$s = 1$	$s = -1$
1	0.9987663	0.9987654	0.9987658
2	3.98026	3.98020	3.98021
3	8.90007	8.89945	8.89950
4	15.6842	15.6799	15.6808
5	24.2289	24.2055	24.2145
—	—	25.0998	—
6	34.4011	34.3599	34.3597
7	46.04	45.94	45.92
—	—	—	51.74
8	58.95	58.70	58.75
9	72.91	72.16	72.41
—	—	74.98	—
10	87.66	86.77	86.59
—	—	—	94.17
11	102.9	101.1	101.3
—	—	110.4	—
12	118.4	115.2	115.2
—	—	—	124.1
13	133.8	127.8	128.3
—	—	134.2	—
14	148.7	140.0	138.7
—	—	—	141.5
15	162.5	146.3	146.7

Table 2: $q = 10^{-2}$. The last two columns show numerical results for $(L/\pi)^2$ times the 19 lowest positive eigenenergies under the boundary condition (5.2) with $s = \pm 1$. The perturbative eigenenergies E_m^{pert} (5.4d), shown in the second column, provide a good approximation to 15 of the eigenenergies, with $1 \leq m \leq 15$, both for $s = 1$ and for $s = -1$, to five decimal places near the lower end and to 10% near the upper end. For each of $s = 1$ and $s = -1$, there are four eigenenergies are not close to E_m^{pert} , and these four nonperturbative eigenenergies intercalate between the perturbative ones differently for $s = 1$ and $s = -1$.

$$q = 10^{-4}$$

m	$L^2 E_m^{\text{pert}}/\pi^2$	$s = 1$	$s = -1$
1	0.999999876629944986	0.999999876629936463	0.999999876629936465
2	3.999998026079120	3.999998026078571	3.999998026078574
3	8.999990007025544	8.999990007019330	8.999990007019331
\vdots	\vdots	\vdots	\vdots
17	288.9896960096	288.9896958038	288.9896958039
—	—	314.6674566416	—
18	323.9870491051	323.9870488796	323.9870488152
\vdots	\vdots	\vdots	\vdots
59	3479.505081	3479.504721	3479.504700
—	—	—	3495.371306
60	3598.401124	3598.400726	3598.400731
\vdots	\vdots	\vdots	\vdots
81	6555.689324	6555.686871	6555.686914
—	—	6672.077214	—
82	6718.422171	6718.419579	6718.419577
\vdots	\vdots	\vdots	\vdots
99	9789.149121	9789.141082	9789.140921
—	—	—	9844.787186
100	9987.662994	9987.654463	9987.654503

Table 3: $q = 10^{-4}$. As in Table 2, for the 102 lowest positive eigenenergies, suppressing the ranges of m where the pattern continues in a straightforward way. Apart from the two nonperturbative eigenenergies for each s , E_m^{pert} (5.4d) is accurate to 11 decimal places near the lower end and to five decimal places near the upper end.

We further showed that this subfamily is unique, subject to certain technical assumptions. The closeness holds individually for each of the perturbative eigenvalues, but we did not attempt to give the closeness a sense that would be valid uniformly over the full set of eigenvalues. It might be possible to characterise this closeness in terms of the topology in which the perturbed time evolution operator converges to the unperturbed one, but such an analysis would require a better control over the global properties of the perturbed spectrum.

The physical motivation to consider a Hamiltonian with the p^3 correction term was that this term may model low energy effects due to quantum gravity [1]. Our main result shows that the quantum theory in the presence of this term can be formulated on the interval so as to be unitary and perturbatively close to the uncorrected particle with the Dirichlet boundary conditions. The special interest of the Dirichlet conditions here is that they can be regarded as generic in the uncorrected theory when the two ends of the interval are considered to be independent of each other [14].

Finally, we saw that the eigenenergies in our near-Dirichlet theories depend on the coefficient of the p^3 term through positive integer and half-integer powers, without rapid oscillations or other signs of irregularity. Our near-Dirichlet boundary conditions hence do not single out for this coefficient discrete values that could be regarded as a quantisation condition on the length of the interval in terms of the underlying quantum gravity scale [4].

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A Appendix: Subspaces of self-adjointness

In this appendix we perform the maximal linear subspace analysis that leads to the self-adjointness boundary conditions (2.8) in the main text.

A.1 Preliminaries

Let n be a positive integer and $\mathcal{H} = \mathbb{C}^{2n}$. Define on \mathcal{H} the Hermitian form

$$B(u, v) = u^\dagger \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} v, \quad (\text{A.1})$$

where I is the $n \times n$ identity matrix.

Lemma. The maximal linear subspaces $V \subset \mathcal{H}$ on which $B(u, v) = 0$ for all $u, v \in V$ are

$$V_U = \{v \in \mathcal{H} \mid \begin{pmatrix} U & -I \\ 0 & 0 \end{pmatrix} v = 0\} , \quad (\text{A.2})$$

where $U \in U(n)$.

Proof. Let $V \subset \mathcal{H}$ be a linear subspace on which $B(u, v) = 0$ for all $u, v \in V$. Suppose $w = \begin{pmatrix} w_1 \\ w_2 \end{pmatrix} \in V$ where $w_1, w_2 \in \mathbb{C}^n$. Then $B(w, w) = 0$ implies $\|w_1\| = \|w_2\|$. As V is a linear subspace, each $v \in V$ must hence have the form $\begin{pmatrix} v_1 \\ Uv_1 \end{pmatrix}$, where U is a constant $n \times n$ matrix, such that if $V_1 \subset \mathbb{C}^n$ denotes the projection of V to its first n components, U maps V_1 isometrically to \mathbb{C}^n . For $u = \begin{pmatrix} u_1 \\ Uu_1 \end{pmatrix}$ and $v = \begin{pmatrix} v_1 \\ Uv_1 \end{pmatrix}$ in V , $B(u, v) = 0$ is equivalent to $u_1^\dagger (U^\dagger U - I) v_1 = 0$. This holds for all $u_1, v_1 \in \mathbb{C}^n$ iff $U^\dagger U = I$. ■

Remark. The maximal linear subspaces on which $B(v, v) = 0$ coincide with (A.2). The proof is as above but setting at every step $u = v$.

For generalisations, see [17, 18].

A.2 Main proposition

Let n be a positive integer and $\mathcal{H} = \mathbb{C}^{2n}$. Define on \mathcal{H} the Hermitian form

$$C(u, v) = u^\dagger A v , \quad (\text{A.3})$$

where A is a Hermitian $2n \times 2n$ matrix with n strictly positive eigenvalues and n strictly negative eigenvalues (each eigenvalue counted with its multiplicity). By matrix diagonalisation, there exists a unitary $2n \times 2n$ matrix P and a real diagonal positive definite $2n \times 2n$ matrix D such that

$$A = (DP)^\dagger \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} (DP) . \quad (\text{A.4})$$

Proposition. The maximal linear subspaces $V \subset \mathcal{H}$ on which $C(u, v) = 0$ for all $u, v \in V$ are

$$V_U = \{v \in \mathcal{H} \mid \begin{pmatrix} U & -I \\ 0 & 0 \end{pmatrix} (DP)v = 0\} , \quad (\text{A.5})$$

where $U \in U(n)$.

Proof. Follows from the Lemma by observing that $C(u, v) = B(DPu, DPv)$. ■

A.3 Application

We specialise (A.3) to

$$A = \begin{pmatrix} G & 0 \\ 0 & -G \end{pmatrix} \quad (\text{A.6})$$

where G is a Hermitian 3×3 matrix with the eigenvalues $\lambda_- < 0$, $\lambda_+ > 0$ and $\lambda_0 > 0$ and the corresponding orthogonal normalised eigen-covectors

$$\begin{pmatrix} a_1 & a_2 & a_3 \end{pmatrix}, \quad \begin{pmatrix} b_1 & b_2 & b_3 \end{pmatrix}, \quad \begin{pmatrix} c_1 & c_2 & c_3 \end{pmatrix}. \quad (\text{A.7})$$

The matrix

$$\tilde{P} = \begin{pmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \\ c_1 & c_2 & c_3 \end{pmatrix} \quad (\text{A.8})$$

is then unitary, and

$$\begin{pmatrix} \tilde{P} & 0 \\ 0 & \tilde{P} \end{pmatrix} A \begin{pmatrix} \tilde{P}^\dagger & 0 \\ 0 & \tilde{P}^\dagger \end{pmatrix} = \text{diag}(\lambda_-, \lambda_+, \lambda_0, -\lambda_-, -\lambda_+, -\lambda_0). \quad (\text{A.9})$$

Let

$$Q = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \quad (\text{A.10})$$

$$\tilde{D} = \begin{pmatrix} \sqrt{-\lambda_-} & 0 & 0 \\ 0 & \sqrt{\lambda_+} & 0 \\ 0 & 0 & \sqrt{\lambda_0} \end{pmatrix}. \quad (\text{A.11})$$

Then (A.4) holds with

$$DP = \begin{pmatrix} \tilde{D} & 0 \\ 0 & \tilde{D} \end{pmatrix} Q \begin{pmatrix} \tilde{P} & 0 \\ 0 & \tilde{P} \end{pmatrix}. \quad (\text{A.12})$$

Writing in (A.5)

$$v = \begin{pmatrix} \rho_1 \\ \rho_2 \\ \rho_3 \\ \sigma_1 \\ \sigma_2 \\ \sigma_3 \end{pmatrix}, \quad (\text{A.13})$$

we have

$$DP \begin{pmatrix} \rho_1 \\ \rho_2 \\ \rho_3 \\ \sigma_1 \\ \sigma_2 \\ \sigma_3 \end{pmatrix} = \begin{pmatrix} \sqrt{-\lambda_-} (a_1 \sigma_1 + a_2 \sigma_2 + a_3 \sigma_3) \\ \sqrt{\lambda_+} (b_1 \rho_1 + b_2 \rho_2 + b_3 \rho_3) \\ \sqrt{\lambda_0} (c_1 \rho_1 + c_2 \rho_2 + c_3 \rho_3) \\ \sqrt{-\lambda_-} (a_1 \rho_1 + a_2 \rho_2 + a_3 \rho_3) \\ \sqrt{\lambda_+} (b_1 \sigma_1 + b_2 \sigma_2 + b_3 \sigma_3) \\ \sqrt{\lambda_0} (c_1 \sigma_1 + c_2 \sigma_2 + c_3 \sigma_3) \end{pmatrix}, \quad (\text{A.14})$$

and the subspace condition (A.5) reads

$$U \begin{pmatrix} \sqrt{-\lambda_-} (a_1 \sigma_1 + a_2 \sigma_2 + a_3 \sigma_3) \\ \sqrt{\lambda_+} (b_1 \rho_1 + b_2 \rho_2 + b_3 \rho_3) \\ \sqrt{\lambda_0} (c_1 \rho_1 + c_2 \rho_2 + c_3 \rho_3) \end{pmatrix} = \begin{pmatrix} \sqrt{-\lambda_-} (a_1 \rho_1 + a_2 \rho_2 + a_3 \rho_3) \\ \sqrt{\lambda_+} (b_1 \sigma_1 + b_2 \sigma_2 + b_3 \sigma_3) \\ \sqrt{\lambda_0} (c_1 \sigma_1 + c_2 \sigma_2 + c_3 \sigma_3) \end{pmatrix}. \quad (\text{A.15})$$

This is the condition (2.8) in the main text.

B Appendix: Small q expansions of the eigenvalues and eigen-covectors

In this appendix we give the small q expansions of the eigenvalues and $\sqrt{|\lambda|}$ times the normalised eigen-covectors (2.6) of the matrix (2.3). The phases of the eigen-covectors are chosen so that $a_1 > 0$, $b_1 > 0$ and $c_3 > 0$.

$$\lambda_- = -1 + \frac{1}{2}q - \frac{5}{8}q^2 - \frac{1}{2}q^3 - \frac{7}{128}q^4 + \frac{1}{2}q^5 + \frac{675}{1024}q^6 + O(q^8) \quad (\text{B.1a})$$

$$\lambda_+ = 1 + \frac{1}{2}q + \frac{5}{8}q^2 - \frac{1}{2}q^3 + \frac{7}{128}q^4 + \frac{1}{2}q^5 - \frac{675}{1024}q^6 + O(q^8) \quad (\text{B.1b})$$

$$\lambda_0 = q^3 (1 - q^2 + 3q^6 + O(q^8)) \quad (\text{B.1c})$$

$$\sqrt{-\lambda_-} a_1 = \frac{1}{\sqrt{2}} \left(1 + \frac{3}{16}q^2 - \frac{83}{512}q^4 + \frac{3605}{8192}q^6 + \frac{1}{2}q^7 + O(q^8) \right) \quad (\text{B.2a})$$

$$\begin{aligned} \sqrt{-\lambda_-} a_2 = & -\frac{i}{\sqrt{2}} \left(1 - \frac{1}{2}q - \frac{3}{16}q^2 - \frac{3}{32}q^3 + \frac{101}{512}q^4 + \frac{595}{1024}q^5 + \frac{4035}{8192}q^6 \right. \\ & \left. - \frac{10261}{16384}q^7 + O(q^8) \right) \end{aligned} \quad (\text{B.2b})$$

$$\begin{aligned} \sqrt{-\lambda_-} a_3 = & \frac{q}{\sqrt{2}} \left(1 + \frac{1}{2}q - \frac{3}{16}q^2 - \frac{29}{32}q^3 - \frac{411}{512}q^4 + \frac{749}{1024}q^5 + \frac{21955}{8192}q^6 \right. \\ & \left. + \frac{33909}{16384}q^7 + O(q^8) \right) \end{aligned} \quad (\text{B.2c})$$

$$\sqrt{\lambda_+} b_1 = \frac{1}{\sqrt{2}} \left(1 + \frac{3}{16} q^2 - \frac{83}{512} q^4 + \frac{3605}{8192} q^6 - \frac{1}{2} q^7 + O(q^8) \right) \quad (\text{B.3a})$$

$$\begin{aligned} \sqrt{\lambda_+} b_2 = \frac{i}{\sqrt{2}} \left(1 + \frac{1}{2} q - \frac{3}{16} q^2 + \frac{3}{32} q^3 + \frac{101}{512} q^4 - \frac{595}{1024} q^5 + \frac{4035}{8192} q^6 \right. \\ \left. + \frac{10261}{16384} q^7 + O(q^8) \right) \end{aligned} \quad (\text{B.3b})$$

$$\begin{aligned} \sqrt{\lambda_+} b_3 = -\frac{q}{\sqrt{2}} \left(1 - \frac{1}{2} q - \frac{3}{16} q^2 + \frac{29}{32} q^3 - \frac{411}{512} q^4 - \frac{749}{1024} q^5 + \frac{21955}{8192} q^6 \right. \\ \left. - \frac{33909}{16384} q^7 + O(q^8) \right) \end{aligned} \quad (\text{B.3c})$$

$$\sqrt{\lambda_0} c_1 = -q^{7/2} (1 - 2q^2 + q^4 + 7q^6 + O(q^8)) \quad (\text{B.4a})$$

$$\sqrt{\lambda_0} c_2 = iq^{5/2} (1 - q^2 - q^4 + 7q^6 + O(q^8)) \quad (\text{B.4b})$$

$$\sqrt{\lambda_0} c_3 = q^{3/2} (1 - q^2 + 4q^6 + O(q^8)) \quad (\text{B.4c})$$

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